This was taken as evidence that the observation tube in Ref. 2 might "have harbored incipient or diffuse pink afterglow." It is not surprising to find these emissions in the discharge as these emission bands are usually present in auroral afterglows. In order to obtain some information concerning the origin of these bands, it is important to determine their spectral intensity distribution. Unfortunately, this was not done in their work. Furthermore, there is no simple logical reason why the presence of these bands in the discharge may exclude their presence in the afterglow, especially in experiments under conditions of high N-atom concentrations where the contribution due to excited species is important.

Brennen and Shuman also suggested that several features present in Fig. 1b of Ref. 1 and Fig. 1 of Ref. 2 might be identified as bands in the N_2 second positive ($2P$) and N_2^+ first negative ($1N$) systems, both of which were considered "telltale diagnostics" of the pink afterglow. They have apparently not considered studies by various workers who have detected these emissions in a variety of N_2 afterglows.[3-5] In fact, we have recently observed emissions due to $N_2(2P)$, $N_2^+(1N)$ and Goldstein–Kaplan bands as well as the 5577 Å and 3466 Å lines in the yellow N_2 afterglow. The intensity distributions of these band systems were found to be quite different from those reported in other afterglows. Kinetic studies on the emission properties indicate that these emission bands, somewhat resembled the highly vibrational bands of $N_2(1P)$ system, develop principally in the observation vessel as a consequence of complex interactions between energetic species.

The pink afterglow was normally observed in our system at pressures between 5 and 15 Torr and at a flow time of a few msec after the discharge. The glow was well isolated from the discharge and the subsequent yellow afterglow, and had a lifetime of a few msec, all of which are very similar to the pink afterglow originally described by Beale and Broida.[6] We are quite confused by Brennen and Shuman's statement that "We have sometimes seen the pink afterglow diffusely distributed throughout the entire volume of our observation tube." If it is implied that the pink glow they observe simply survived from the discharge, how do they explain the mean halflife of the order of 10^{-3} sec estimated by Beale and Broida, and others? On the other hand, if the pink afterglow is created by active species in the observation vessel, how shall we define the pink afterglow? Interactions involving energetic species under conditions of high atom concentrations are undoubtedly complicated. Argument over classical characterization of afterglows of this nature may serve little purpose. Our present interest is simply to try to understand the general nature of energy transfer processes involving energetic species in the long-lived yellow afterglow of nitrogen.

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Comment on "Theory of collisions between an atom and a diatomic molecule in the body-fixed coordinate system"[a)]

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In two recent papers,[1,2] Choi, Poe, and Tang (CPT) have presented a theory of atom–diatom nonreactive scattering using body fixed (BF) coordinates which is quite similar to a theory previously developed[3] and used[4] by us in applications to the $H + H_2$ reaction. In comparing their and our asymptotic scattering matrix solutions, CPT noted that our lacked a phase factor i^{J+j+15} and further stated[1] that "erroneous numerical results could be introduced by omitting this phase factor." We show here that, contrary to this statement, this phase factor difference *does not* cause our results to be in error. In addition, we point out that CPT misquoted our conclusions concerning the Ω dependence of the $H + H_2$ rotationally inelastic nonreactive transition probabilities.

CPT's argument concerning phase factors is based on the following asymptotic form for the BF S-matrix so-

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lution, which they derived by a unitary transformation on the corresponding space fixed (SF) solution[1] (expressed in the quantum number notation of Eq. (5.3) of Ref. 3,[5] and ignoring closed channels which are not essential here):

$$\Psi^{v'j'\Omega'}_{JM}[S] \underset{R\to\infty}{\sim} \sum_{vj\Omega} D^{J}_{M\Omega}(\phi,\theta,0)Y_{j\Omega}(\gamma,\psi)\frac{\phi_{vj}(r)}{rR}\, b^{v'j'\Omega'}_{Jvj}[S]\,, \tag{1}$$

where

$$b^{v'j'\Omega'}_{Jvj}[S] = 2\pi i^{J+j+1}\left(\frac{k_{v'j'}}{k_{vj}}\right)^{1/2}\{\exp[-i(k_{vj}R-(J+j)\pi/2)]\,\delta^{v'j'\Omega'}_{vj\Omega} - S^{v'j'\Omega'}_{Jvj\Omega}\exp[i(k_{vj}R-(J+j)\pi/2)]\}\,, \tag{2}$$

and $S^{v'j'\Omega'}_{Jvj\Omega}$ is CPT's scattering matrix.[6] Except for an unimportant $2\pi(V_{v'j'})^{1/2}$ factor, Eq. (2) differs only by the phase factor i^{J+j+1} from an analogous expression used by us[3] [Eq. (5.5) of Ref. 3], by Pack,[7] and by Walker and Light[8] to define a scattering matrix (which we denote here as $S^{v'j'\Omega'}_{Jvj\Omega}$). CPT argued[1] that because the quantum number j is summed over in Eq. (1), a wave function $\Psi^{v'j'\Omega'}_{JM\Omega}[S]$ obtained from an expression without the i^{J+j+1} factor will be different than one with it, presuming that the same S matrix is used in both solutions. They further argued that this "phase factor has nothing to do with the definition of the S matrix," implying that the same S matrix would be obtained with either solution.

We will now show that this last statement is, in fact, incorrect, and that the S matrix obtained using our asymptotic solution differs from theirs by a phase factor $i^{j-j'}$. To prove this, we examine the incoming spherical wave parts of both solutions. In Eq. (2) that is

$$\Psi^{v'j'\Omega'}_{JM}[S]_{\rm inc} \underset{R\to\infty}{\sim} D^{J}_{M\Omega'}(\phi,\theta,0)Y_{j'\Omega'}(\gamma,\phi)\,\frac{\phi_{v'j'}(r)}{rR} \times 2\pi\left(\frac{k_{v'j'}}{k_{vj}}\right)^{1/2} i^{J+j'+1}\exp[-i(k_{v'j'}R-(J+j)\pi/2)]\,, \tag{3}$$

while ours is identical to Eq. (3) except for the $i^{J+j'+1}$ factor (and the unimportant $2\pi(V_{v'j'})^{1/2}$). This means that the CPT incident solution equals $i^{J+j'+1}$ times our incident solution. Since both solutions solve the same Schrödinger equation,[9] this same factor must likewise relate the outgoing wave solutions, and this implies (equating coefficients of corresponding terms) that,

$$i^{J+j'+1}S^{v'j'\Omega'}_{Jvj\Omega} = i^{J+j+1}S^{v'j'\Omega'}_{Jvj\Omega}\,, \tag{4}$$

or

$$S^{v'j'\Omega'}_{Jvj\Omega} = i^{j-j'}S^{v'j'\Omega'}_{Jvj\Omega}\,. \tag{5}$$

It is now clear that CPT's S-matrix solution [Eq. (1)] and ours differ only by the *multiplicative* phase factor $i^{J+j'+1}$ (note the presence of j' rather than j in this factor), and this cannot have any measurable consequence. We should note that the factor $i^{j-j'}$ in Eq. (5) can also be derived by comparing scattering amplitudes [using CPT's Eq. (28) and our Eq. (5.31)[10]], or by comparing the relationship between BF and space fixed (SF) scattering matrices [CPT's Eq. (21) and our Eq. (5.14)[11]]. CPT do correctly point out that their BF R matrix boundary conditions (and wave functions) are, "completely different," from ours. This is, of course, not surprising since their BF R and S matrices are not related by the same equation (Eq. (30) of Ref. 1) as ours [Eq. (5.7) of Ref. 3]. This difference does not affect any observable properties such as transition probabilities or cross sections, since these are defined in terms of the S matrix, (i.e., plane wave) solution.

Finally, we note that in examining transition probabilities for rotationally inelastic nonreactive $H+H_2$ collisions, CPT improperly attributed to us[12] the conclusion that (quoting from Ref. 2), "for low J, the K values are conserved approximately in closed-coupling

TABLE I. Comparison of rotationally inelastic transition probabilities $P^{02\Omega'}_{J04\Omega}$ for nonreactive $H+H_2$,[a] $J=15$.

	CPT[b] at $E=0.673$ eV			SK[c] at $E=0.70$ eV		
Ω \ $-\Omega'$	0	1	2	0	1	2
−4	2.397(−3)	6.423(−4)	5.551(−5)	2.900(−3)	6.614(−4)	1.326(−5)
−3	2.434(−3)	8.660(−4)	1.782(−4)	2.805(−3)	7.493(−4)	3.039(−4)
−2	5.343(−3)	9.676(−4)	2.115(−4)	7.225(−3)	9.577(−4)	1.595(−4)
−1	7.949(−3)	2.876(−3)	3.834(−4)	9.813(−3)	3.671(−3)	4.236(−4)
0	1.060(−2)	4.992(−3)	1.019(−3)	1.399(−2)	6.562(−3)	1.203(−3)
1	7.949(−3)	8.916(−3)	2.255(−3)	9.813(−3)	1.167(−2)	2.925(−3)
2	5.343(−3)	8.838(−3)	5.851(−3)	7.225(−3)	1.093(−2)	7.992(−3)
3	2.434(−3)	4.950(−3)	9.891(−3)	2.805(−3)	6.255(−3)	1.296(−2)
4	2.397(−3)	6.128(−3)	6.046(−3)	2.900(−3)	7.798(−3)	7.333(−3)

[a] 2.397(−3) should be read as 2.397×10^{-3}, etc.
[b] Reference 2.
[c] These results were generated as part of the calculations described in Ref. 4, although they have not previously been published.

calculations and dominant contributions of transition probabilities are from $K_\beta = K_\alpha = 0$," (i. e., $\Omega = \Omega' = 0$). They proceeded to challenge this statement as if it had been made for nonreactive scattering. In Ref. 12 we did make a statement similar to this, but it refers specifically to *reactive* scattering (in $H + H_2$). Our conclusion for *nonreactive* scattering was discussed thoroughly in Ref. 4, where we stated, "An examination of other nonreactive transition probabilities indicates no strong tendency for a $m_j = -m_{j'}(\Omega = \Omega')$ "j_z-conserving" selection rule as has been assumed in rotationally inelastic scattering." In fact, there is no essential difference between the Ω, Ω' dependence of CPT's transition probabilities and ours. We demonstrate this in Table I[13] for the $j = 2$ to $j' = 4$ transition.

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[b]Contribution No. 5890.

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[6]Note that $\bar{S}^{v'j'\Omega'}_{Jvj\Omega}$ here would have been labelled as $\bar{S}^{vj\Omega}_{Jv'j'-\Omega'}$ in Eq. (5.5) of Ref. 3.
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[9]CPT argued[1] that $\Psi^{v'j'\Omega'}_{JM}[S]$ in Eqs. (1) and (2) does not solve the BF Schrödinger equation if the i^{J+j+1} is omitted because the BF Hamiltonian does not commute with a diagonal matrix having diagonal elements i^{J+j+1}. Asymptotically, however, the Hamiltonian is *diagonal* in j so their argument does not apply, and both wave functions solve the BF Schrödinger equation in that region. Either solution may furthermore be matched to solutions which solve the Schrödinger equation at small R as shown in detail in Ref. 3 for our solution.
[10]CPT used the same plane wave solution as we, and it is easy to see that the scattering amplitudes are simply proportional. By relating these quantities and using Eq. (28) of Ref. 1 and Eq. (5.31) of Ref. 3, we again derive Eq. (5). Note that the meaning of primed and unprimed quantum numbers in Eq. (5.31) is reversed from that used here.
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[13]The actual differences between their and our transition probabilities in Table I are probably due to a combination of effects, including the slightly different energies at which the calculations were done, the different vibration-rotation basis sets used, and the different representations of the potential used (CPT truncated the expansion of the potential in Legendre polynomials at the P_2 term while we included the P_4 term.)

On "Theory of collisions between an atom and a diatomic molecule in the body-fixed coordinate system"[a]

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In recent papers with the above titles,[1,2] we presented a detailed formulation for the treatment of *parities* in a body-fixed (BF) close-coupling approximation. This is directly amenable to numerical computation of elastic and inelastic atom-diatom scattering cross sections.

The main thrust of our paper is the parity boundary conditions. However, in the preceding comment by Schatz and Kuppermann, they raised some questions regarding the relationship between the *nonparity* boundary conditions for S matrix developed by us and by them. It seems necessary for us to clarify the implications of some statements which we made about nonparity asymptotic boundary conditions for S matrix, not to be misunderstood by other colleagues in this field who have employed different forms of the boundary condition from ours. (Hereafter, the "asymptotic" will be deleted.)

We stated that if $A^P(R)$ is another boundary condition different from our $A(R)$ defined in Ref. 1 as

$$A_{j_\gamma K_\gamma, j_\alpha K_\alpha}(R) = 2\pi i^{J+j_\gamma+1} \times (\delta_{j_\gamma j_\alpha}\delta_{K_\gamma -K_\alpha} \exp\{-i[k_\gamma R - (J+j_\gamma)\pi/2]\} - \bar{S}^J_{j_\gamma K_\gamma, j_\alpha K_\alpha} \exp\{i[k_\gamma R - (J+j_\gamma)\pi/2]\}), \quad (1)$$

then

$$A^P(R) = PA(R)Q, \quad (2)$$

for some nonsingular matrices P and Q.[3] Here, $A^P(R)$ is an expression in terms of corresponding S matrix

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